Longer/integrative problem (20 points total)

Resources allowed: Appendices *and* your own hand-written class notes only

Good Chemistry—ODEs, PDEs, and Fourier

The problem solves the Diffusion Equation, a partial differential equation that solves everything from temperature "diffusing" in a material, to electrons diffusing in semiconductor material, to molecules diffusing in a fluid. We'll use the last of these as motivation for this problem, as it is most intuitive.

Imagine we have a thin tube of length L, with the central axis oriented along the x-axis. We'll just tackle the 1-dimensional diffusion equation for now (ignoring whether the tube has a rectangular, or circular cross-section). We'll imagine that the tube is full of saline solution and that we'll inject a tiny drop of colored dye into the tube. We want to solve the for $C(x,t)$, the dye concentration in the tube as a function of position and time. (Of course this could be oxygen concentration in a combustion engine cylinder; or a drop of intravenous medicine in a blood stream, etc.)

OK, now the specifics. The ***diffusion equation*** describes how the dye concentration evolves over space and time, and is given by:

$$\frac{1}{\alpha^2}\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t}$$

In lay language this says that the dye concentration at a certain location decreases in time if the concentration profile at a particular time has a negative curvature, as would be the situation illustrated in Figure 1 near $x = w$. The positive real constant α^2 expresses how easy easy it is for the dye to move through the fluid: the smaller the value of α, the easier it is for the dye to diffuse; and vice-versa.

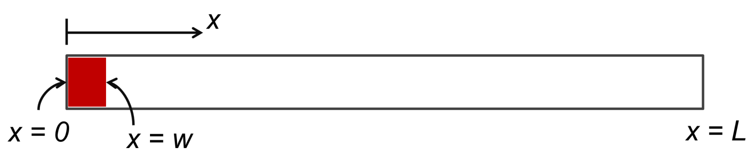

Figure 1: Cartoon illustration of thin tube of length L loaded with initial drop of dye depicted as red color.

Our ***boundary conditions*** are that there can be no flux through the end caps. This is expressed, not as the concentration itself, but using the first partial derivative with respect to x as follows:

$$\frac{\partial C}{\partial x}(x=0,t) = 0; \qquad \frac{\partial C}{\partial x}(x=L,t) = 0$$

1. Use the separation of variables technique to show that the concentration as a function of time is given by:

$$C(x,t) = \sum_{n=0}^{\infty} A_n \cos(\alpha k_n x) e^{-k_n^2 t} \tag{1}$$

   where $k_n = \frac{n\pi}{\alpha L}$.

2. Sketch the first 4 spatial modes allowed as part of the solution, i.e. the function $\cos(\alpha k_n x)$ for $n = 0, 1, 2, 3$.

3. Note the summation in Eqn 1 begins at $n = 0$. Physically what does this mean? Argue why this is a valid mode (contrasted with the the $n = 1$ indexing we've seen and used so many times working examples in class).

4. Let's assume a small drop of dye is introduced to the left side of the tube as depicted in Figure 1. Thus, the ***initial condition*** is given by:

$$C(x, t = 0) = C_o \text{ for } x \leq w; \qquad C(x, t = 0) = 0 \text{ for } x > w$$

   Intuitively, what will be the steady state-concentration profile of dye in the tube after waiting for a very long time? Sketch your solution for $C(x, t)$ for $t \to \infty$.

5. Now derive an expression for the coefficients A_n in Eqn 1 in terms of α, n, L, w, and C_o. Hint: be careful to appropriately handle the $n = 0$ case.

6. Show/argue that your full-on PDEs solution agrees with the intuitive solution the long-term steady state solution of concentration as a function of position.

7. Extra credit!! Assume $L = 10$ cm; $w = 1/2$ cm; $\alpha^2 = 4$ s/cm^2; and $C_o = 1$ M. Make a sketch of $C(x, t)$ for $x = [0, L]$ at time pints $t = 0, 1, 10, 1000$ s. That is, sketch 4 successive snapshots of the concentration of dye in the tube at the prescribed times. Provide brief rationale justifying your hand-sketch snapshots.